

1,4-Diazabicyclo[2.2.2]octane
280-57-9 | DTXSID0022016

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: -0.149

Global applicability domain: Inside

Local applicability domain index: 5.04e-01

Confidence level: 6.57e-01

Nearest Neighbors from the Training Set

Image not found

1,2-Ethanediamine, N,N,N'-trimethyl-

Measured: -0.200

Predicted: -0.197

Image not found

1,1,3,3-Tetramethyl-2-thiourea

Measured: 0.49

Predicted: 3.20e-01

Image not found

1,4-Dimethylpiperazine

Measured: -0.400

Predicted: -0.238

Image not found

N-Methylhomopiperazine

Measured: -0.400

Predicted: -0.265

Image not found

4-Methylmorpholine

Measured: -0.330

Predicted: -0.246